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In Situ X-ray Standing Wave Atomic-scale 3-D Imaging of Catalysts Supported on Oxide: VO_x/α-TiO_2 (110)

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Supported vanadia on oxides are important catalysts. If the atomic-scale surface structure of VO_x could be predicted, this would impact our understanding of numerous chemical processes. Thus, atomic layer deposition-grown VO_x on rutile (110) was used for finding the positions of vanadium (V) with respect to the support lattice and its sensitivity to the reduction-oxidation (redox) cycle. *In situ* x-ray standing waves (XSW) are used to determine the structure changes during the redox reaction. The results for 3/4 ML V show that V cations on the surface have different structures in the oxidized and reduced states. The 3-D atomic density maps created from XSW measurements show V cations surface site locations directly. X-ray photoelectron spectroscopy is used to correlate the V oxidation state(s) with the above redox induced structural changes. A model is proposed to explain the reversible geometrical/electronic structure changes during this redox reaction. With this model-dependent analysis, it shows that V at atop sites mainly participated in the redox reactions, indicating a top site could be a catalytic active site. The reversibility in redox reactions implies the important application in catalysis.